Method and System for Predicting
Pharmacokinetic Properties
Mamoru Uchiyama, et al.
09/876,767

OIPE JC173
SEP 1 7 2004
PATENT & TRADEMARK OFFICE

(a) Preparation of 2D
structure of molecule

(b) Generaiton and storage
of 2D-fingerprint

Predefined table of
substructures

Internally developed
SPL code

(c) Correlation analysis to
yield QSPR model

PK related Data
ex. T1/2, %HIA, Caco-2
permeability, B/P ratio

trial molecules

(d) Prediction of PK
property

Fig.1

Method and System for Predicting
Pharmacokinetic Properties
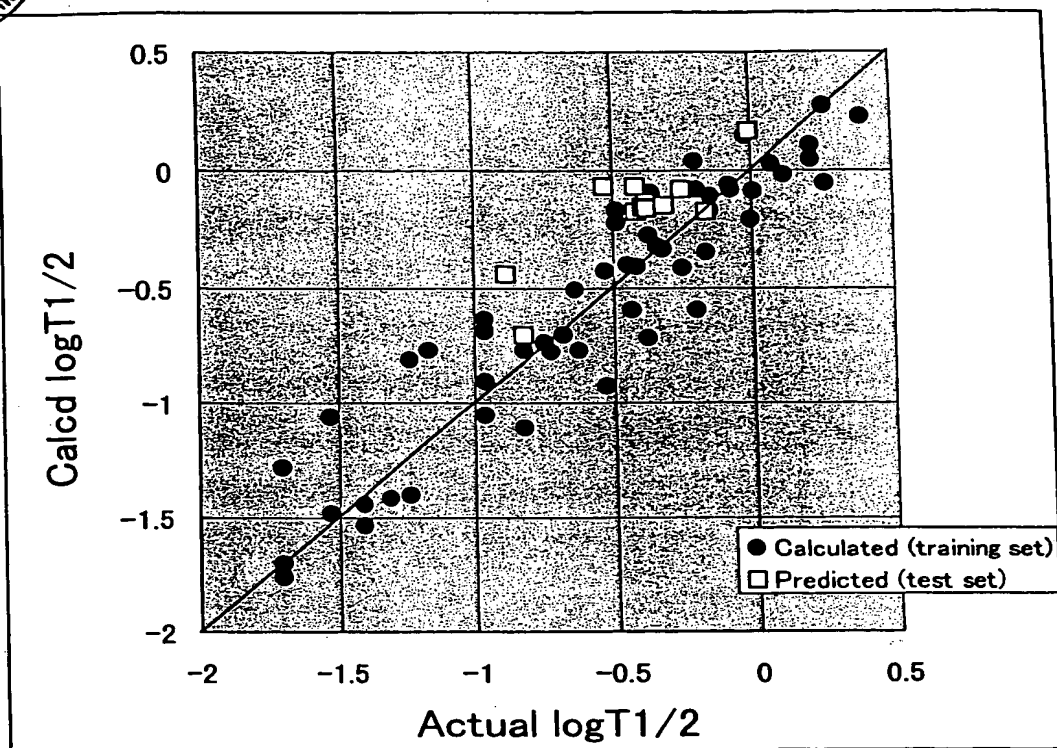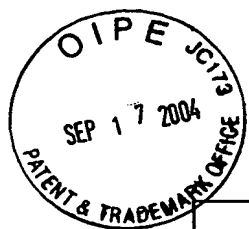Mamoru Uchiyama, et al.
09/876,767

Fig. 2.   Calculated *vs.* actual log t1/2.

Calculated values for training set (N = 54) are indicated as closed circles and predicted values for test set as open squares.
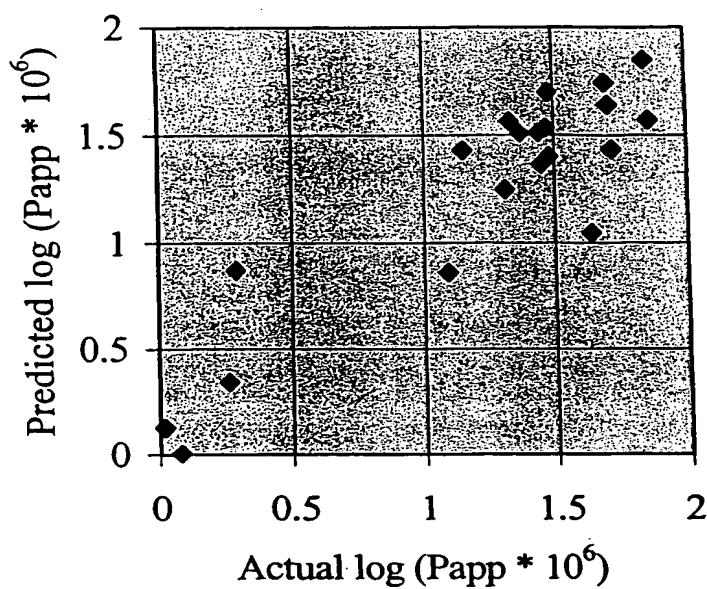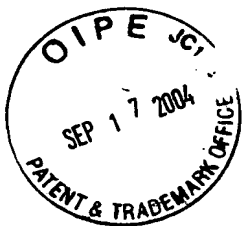
Method and System for Predicting
Pharmacokinetic Properties
Mamoru Uchiyama, et al.
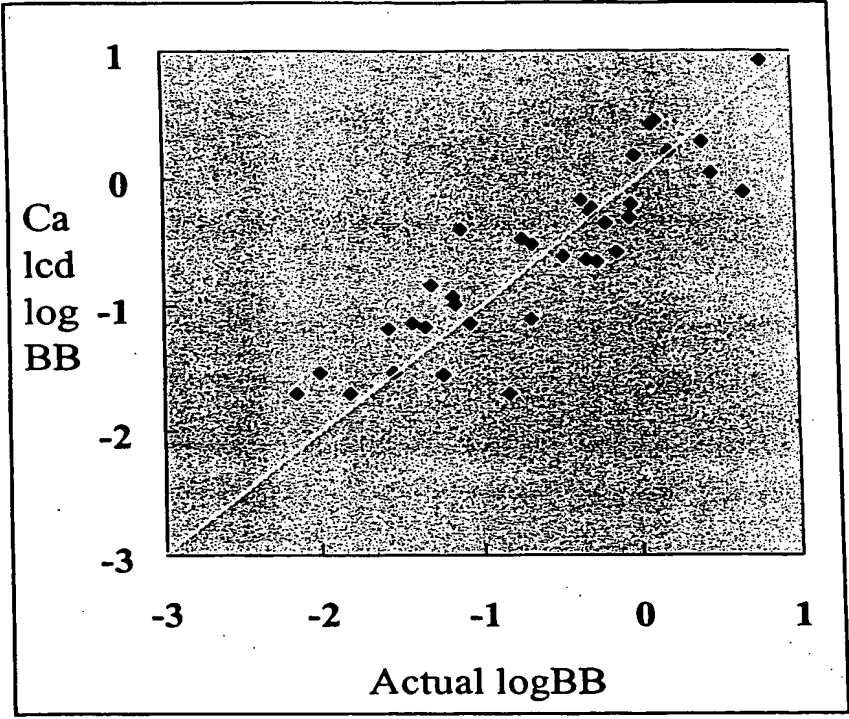09/876,767

Fig. 3.   Calculated *vs.* actual log(P_{app} * 10^6).

Fig. 4. A plot of actual vs. calcd logBB.